

Thermal quantum discord in the Heisenberg chain with impurity

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We study thermal quantum discord (TQD) in the Heisenberg chain with spin site or magnetic impurity. The former one of which may induce inhomogeneous exchange interactions between the neighboring spins, while the latter one modelling a spin chain with nonuniform magnetic field. In contrast with one's traditional understanding, we found that the spin impurity can be used to enhance the TQD greatly for all the bipartition schemes of the chain, while the magnetic impurity located on one spin can make the TQD between the other two spins approaching its maximum 1 for the antiferromagnetic chain.

PACS numbers: 03.65.Ud, 03.65.Ta, 03.67.Mn

Key Words: Thermal quantum discord; Impurity; Heisenberg chain

I. INTRODUCTION

The distinctive features of quantum mechanics qualifies one to carry out many information processing tasks which cannot be done in a classical way [1–7]. The existence of quantum correlations in a system was considered to be responsible for the advantage of this way of information processing [8], and this makes the quantification and understanding of quantum correlations a vital problem needs to be solved.

For a long time, the study of quantum correlations are focused on entanglement [8], which has been shown to be a precious resource in quantum information processing (QIP), and entanglement exists only in non-separable states. But recent studies revealed that quantumness other than entanglement can also exists in separable states [9]. Particularly, there are quantum algorithms which outperform their classical counterparts while with vanishing or negligible entanglement [10]. It is assumed that quantum discord (QD) [11], a more fundamental measure of quantum correlation than that of entanglement, provides speedup for this task.

Due to the role it played in QIP [12–15], and its fundamentals in quantum mechanics [16–18], QD has become one of people's research focuses in recent years [19–23]. Particularly, as a natural candidate for implementing QIP tasks, the spin-chain systems have attracted researcher's great interests, and the behaviors of QD in various spin chains were analyzed [24–29]. More importantly, it has been found that the QD can serve as an efficient quantity for detecting critical points of quantum phase transitions even at finite temperature [16, 30, 31], while the entanglement cannot achieve the same feat.

Different from previous studies which focused on QD behaviors in the spin chain with only homogeneous exchange interactions [24–29], here we go one step further and consider QD behaviors in the Heisenberg model with inhomogeneous interactions. This model can be viewed as a spin chain with spin site imperfection or impurity [32, 33], and the strength of interactions between the impurity spin and its neighboring spins can be different from that between the nor-

mal spins. Here, we will show that while being considered to be an unwanted effects traditionally, the spin impurity can also serve as an efficient way for controlling QD. Particularly, states with considerable amount of QD exists in a wide regime of the spin-impurity-induced inhomogeneous interaction, and this shows the positive side of this unwanted effects.

Besides spin impurity, we will also consider the effect of a nonuniform magnetic field on QD in the Heisenberg model. This model describes the situation in which a magnetic impurity is located on one site of the chain, and the entanglement properties in a similar but different model (i.e., XX chain) has already been discussed [34]. Here, we will further show that if the magnetic impurity is located on the spin which is being traced out, then the QD between the other two spins can be enhanced asymptotically to its maximal value 1 for the antiferromagnetic chain.

The structure of the following text is organized as follows. In Section II, we give a brief review of QD and its quantification based on the discrepancy between two expressions of mutual information extended from classical to quantum system. Then in Sections III and IV, we introduce the spin model we considered and discuss QD behaviors under different system parameters. Finally, we conclude this work with a summary of the main finding in Section V.

II. BASIC FORMALISM OF QD

We recall in this section some basic formalism for QD. Up to now, many measures of QD have been proposed, and they can be classified into two categories in general [9]. The first category are those based on the entropic quantities [11, 35–37], while the second category are defined via the geometric approach based on different distance measures [38–40]. We adopt in this work the original definition of QD proposed by Ollivier and Zurek [11]. If one denotes the quantum mutual information for a bipartite density matrix ρ_{AB} as $I(A : B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB})$, then the QD can be defined as

$$D(\rho_{AB}) = I(A : B) - J(\rho_{AB}), \quad (1)$$

where $J(\rho_{AB})$ is the so-called classical correlation of the following form [41]

$$J(\rho_{AB}) = S(\rho_B) - \inf_{\{E_k^A\}} S(B|\{E_k^A\}), \quad (2)$$

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where $S(B|\{E_k^A\}) = \sum_k p_k S(\rho_{B|k})$ represents the average conditional entropy of the postmeasurement state $\rho_{B|k} = \text{Tr}_A(E_k^A \rho_{AB})/p_k$, with $p_k = \text{Tr}(E_k^A \rho_{AB})$ being the probability for obtaining the measurement outcome k , and the positive operator valued measurements are performed on A .

The QD defined above was considered to be potential resource for many QIP tasks [10, 13], but its closed expression can only be obtained for certain special states [42–47], and it has been shown to be an impossible-to-solve problem for general quantum states [48]. Our discussion in this paper deals with only qubit states, thus we can resort to numerical methods, and in view of the generally negligible improvement by doing minimization over full POVMs [49, 50], we restrict ourselves to the projective measurements by choosing the measurement operators as $\Pi_1^A = |k_1^A\rangle\langle k_1^A|$ and $\Pi_2^A = I - \Pi_1^A$, with $k_1^A = \cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle$. Moreover, for the two-qubit X state with elements $\rho_{AB}^{22} = \rho_{AB}^{33}$, the infimum of the conditional entropy in Eq. (2) can be derived as [51]

$$\inf_{\{\theta, \phi\}} S(B|\{E_k^A\}) = H(\tau), \quad (3)$$

with the variable τ in the Shannon entropy function $H(\tau)$ being given by

$$\tau = \frac{1 - \sqrt{[1 - 2(\rho_{AB}^{11} + \rho_{AB}^{33})]^2 + 4(|\rho_{AB}^{14}| + |\rho_{AB}^{23}|)^2}}{2}. \quad (4)$$

Thus both $J(\rho_{AB})$ and $D(\rho_{AB})$ can be derived analytically for this class of states.

III. THE MODEL

We consider in this paper the three-qubit Heisenberg chain in the thermodynamic limit with the imposition of the periodic boundary condition. The first case we will discuss is the chain for which the neighboring spins coupled with inhomogeneous strengths, and the Hamiltonian can be written as

$$\hat{H} = J_1(\vec{\sigma}_1 \cdot \vec{\sigma}_2 + \vec{\sigma}_3 \cdot \vec{\sigma}_1) + J\vec{\sigma}_2 \cdot \vec{\sigma}_3, \quad (5)$$

where $\vec{\sigma}_n = (\sigma_n^x, \sigma_n^y, \sigma_n^z)$ is the vector of Pauli matrices, while J_1 and J are the coupling strengths, and $\hbar = 1$ in Eq. (5) is assumed.

The above model can be viewed as a ring with an spin impurity at site 1. When it is thermalized with an external reservoir at temperature T , the canonical ensemble can be evaluated by the following density matrix,

$$\rho(T) = Z^{-1} \exp(-\hat{H}/k_B T), \quad (6)$$

with $Z = \text{Tr}[\exp(-\hat{H}/k_B T)]$ being the partition function and k_B the Boltzman's constant, which will be set to unity in the following text. As $\rho(T)$ represents a thermal state, the QD in this state is called the thermal quantum discord (TQD) [16].

The eigenvalues as well as the eigenvectors of the Hamiltonian \hat{H} in Eq. (5) can be derived analytically, for which we denote them as ϵ_i and $|\Psi_i\rangle$ ($i = 1, 2, \dots, 8$), respectively. They

are given by $\epsilon_{1,2} = J - 4J_1$, $\epsilon_{3,4} = -3J$, $\epsilon_{5,6,7,8} = J + 2J_1$, and

$$\begin{aligned} |\Psi_1\rangle &= (|101\rangle + |110\rangle - 2|011\rangle)/\sqrt{6}, \\ |\Psi_2\rangle &= (|001\rangle + |010\rangle - 2|100\rangle)/\sqrt{6}, \\ |\Psi_3\rangle &= (|001\rangle - |010\rangle)/\sqrt{2}, \\ |\Psi_4\rangle &= (|101\rangle - |110\rangle)/\sqrt{2}, \\ |\Psi_5\rangle &= (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}, \\ |\Psi_6\rangle &= (|011\rangle + |101\rangle + |110\rangle)/\sqrt{3}, \\ |\Psi_7\rangle &= |000\rangle, |\Psi_8\rangle = |111\rangle. \end{aligned} \quad (7)$$

Then $\rho(T) = \sum_i \exp(-\epsilon_i/T) |\Psi_i\rangle\langle\Psi_i| / \sum_i \exp(-\epsilon_i/T)$. In the next section, we will compute TQD for the density matrices $\rho_{12}(T) = \text{Tr}_3 \rho(T)$, $\rho_{23}(T) = \text{Tr}_1 \rho(T)$, and $\rho(T)$ with the bipartition $\{1-23\}$, and discuss their behaviors for $T \geq 0$ by changing the system parameters.

Besides spin impurity which induces inhomogeneous interactions between the neighboring spins, we consider also the Heisenberg model with a magnetic impurity [34], which modelling a spin chain with nonuniform magnetic field. The corresponding Hamiltonian is given by

$$\hat{H} = J(\vec{\sigma}_1 \cdot \vec{\sigma}_2 + \vec{\sigma}_2 \cdot \vec{\sigma}_3 + \vec{\sigma}_3 \cdot \vec{\sigma}_1) + B\sigma_1^z, \quad (8)$$

where B is the nonuniform magnetic field along z -direction of the first spin.

For this Hamiltonian, its eigenvalues are $\epsilon_{1,2} = 3J \pm B$, $\epsilon_{3,4} = -3J \pm B$, $\epsilon_{5,6} = \pm\eta_+$, and $\epsilon_{7,8} = \pm\eta_-$. Its eigenvectors can also be obtained analytically, which are of the following form

$$\begin{aligned} |\Psi_1\rangle &= |000\rangle, |\Psi_2\rangle = |111\rangle, \\ |\Psi_3\rangle &= (|001\rangle - |010\rangle)/\sqrt{2}, \\ |\Psi_4\rangle &= (|101\rangle - |110\rangle)/\sqrt{2}, \\ |\Psi_{5,6}\rangle &= |001\rangle + |010\rangle - \frac{B + J \mp \eta_+}{2J} |100\rangle, \\ |\Psi_{7,8}\rangle &= |101\rangle + |110\rangle + \frac{B - J \pm \eta_-}{2J} |011\rangle. \end{aligned} \quad (9)$$

where $\eta_{\pm} = \sqrt{B^2 + 9J^2 \pm 2JB}$, and $|\Psi_{5,6,7,8}\rangle$ are unnormalized.

IV. TQD IN THE HEISENBERG CHAIN WITH IMPURITY

The impurity plays an important role in condensed matter physics. We discuss here effects of the spin and magnetic impurities on TQD, and show that while generally being considered to be the unwanted effects, proper engineering of the impurity can also be used to enhance the TQD greatly.

A. Spin impurity

We consider first the case of the spin impurity on TQD. For the reduced density matrices $\rho_{12}(T)$ and $\rho_{23}(T)$, as they are

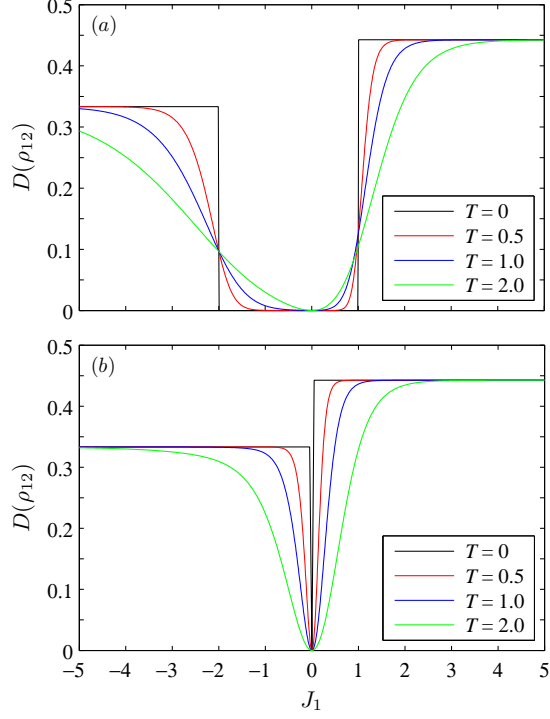


FIG. 1: TQD $D(\rho_{12})$ between spins 1 and 2 versus J_1 with different scaled temperature T , and the parameter J is chosen to be $J = 1$ (a) and $J = -1$ (b), respectively.

X states and satisfy the conditions required by Eq. (3), closed expressions of TQD can be obtained (we do not list them here for concise of the presentation). For $\rho(T)$ with the bipartition $\{1-23\}$, we compute the TQD numerically.

When considering TQD between the impurity spin and the normal spin, the J_1 dependence of $D(\rho_{12})$ with different T are displayed in Fig. 1. First, at absolute zero temperature with $J > 0$, the ground states are the mixtures of $|\Psi_{5,6,7,8}\rangle$ if $J_1 < -2J$, $|\Psi_{3,4}\rangle$ if $J_1 \in (-2J, J)$, and $|\Psi_{1,2}\rangle$ if $J_1 > J$, and the TQDs are given by $1/3$, 0 , and 0.4425 , respectively. When $J < 0$, however, the ground states are the mixtures of $|\Psi_{5,6,7,8}\rangle$ if $J_1 < 0$, which gives $D(\rho_{12}) = 1/3$; and $|\Psi_{1,2}\rangle$ if $J_1 > 0$, which gives $D(\rho_{12}) = 0.4425$.

For finite T , as can be seen from Fig. 1, $D(\rho_{12})$ increases with increasing $|J_1|$, and when $J_1 \rightarrow \infty$ and $-\infty$, we have $D(\rho_{12}) = 0.4425$ and $1/3$, respectively. In order to obtain an intuition about the role of the spin impurity played on enhancing TQD at finite T , we define the critical J_{1c} after which $D(\rho_{12})|_{T=0} - D(\rho_{12})|_{T>0} < 10^{-6}$. The numerical fitting results performed in the region of $T \in (1, 10)$ revealed that if $J > 0$, J_{1c} satisfy the power law $J_{1c} \simeq 3.401T + 1.001$ when $J_1 > J$, and $J_{1c} \simeq -7.450T - 2.001$ when $J_1 < -2J$. Similarly, if $J < 0$, we have $J_{1c} \simeq 3.401T - 0.9846$ when $J_1 > 0$, and $J_{1c} \simeq -7.45T + 1.999$ when $J_1 < 0$.

The above phenomena show that the TQD can be improved greatly compared with that of the homogeneous Heisenberg chain (i.e., $J_1 = J$), and the spin impurity can serve as an efficient way for tuning TQD even at finite temperature. Moreover, it is worthwhile to note that the TQD may be increased

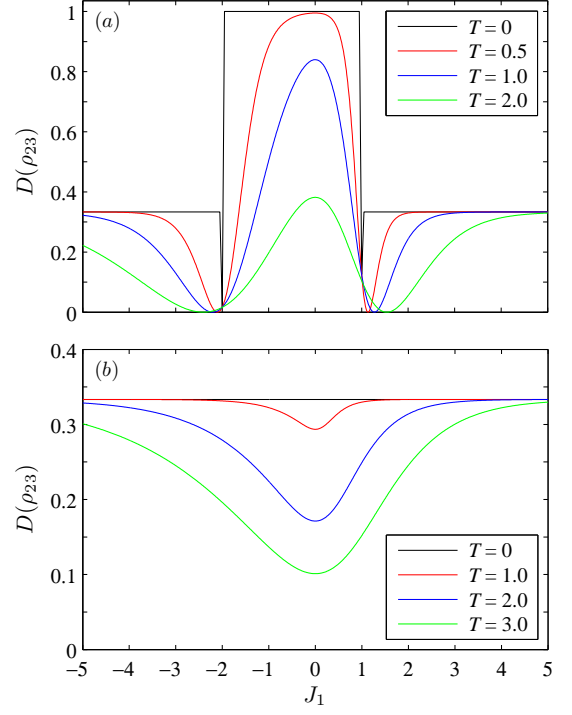


FIG. 2: TQD $D(\rho_{23})$ between spins 2 and 3 versus J_1 with different scaled temperature T , and the parameter J is chosen to be $J = 1$ (a) and $J = -1$ (b), respectively.

by increasing T in the region of $J_1 \in (-2J, J)$ if $J > 0$, and this peculiar phenomenon has also been observed previously when studying entanglement [52, 53].

When considering TQD between the normal spins 2 and 3 at absolute zero temperature with $J > 0$, we have $D(\rho_{23}) = 1/3$ in the regions of $J_1 < -2J$ and $J_1 > J$, and $D(\rho_{23}) = 1$ in the region $J_1 \in (-2J, J)$. The latter case corresponds to mixtures of $|\Psi_3\rangle$ and $|\Psi_4\rangle$, for which ρ_{23} belongs to one of the Bell states and thus the result $D(\rho_{23}) = 1$ is understandable [11]. If $J < 0$, the ground state $\rho_{23} = (|01\rangle + |10\rangle)(\langle 01| + \langle 10|)/6 + (|00\rangle\langle 00| + |11\rangle\langle 11|)/3$ in the full region of J_1 , and thus we always have $D(\rho_{23}) = 1/3$.

At finite temperature, the TQD $D(\rho_{23})$ is reduced with increasing T in a wide regime of J_1 , and the exception appears at the neighborhood of $J_1 > J$ or $J_1 < -2J$ for $J > 0$ (see, Fig. 2). For any fixed T , $D(\rho_{23})$ can be enhanced asymptotically to the steady-state value $1/3$ when $|J_1| \rightarrow \infty$. In fact, for the same defined J_{1c} above with $J > 0$, we have $J_{1c} \simeq 4.245T + 1.001$ when $J_1 > J$, and $J_{1c} \simeq -8.144T - 2.001$ when $J_1 < -2J$. If $J < 0$, we have $J_{1c} \simeq 4.245T - 0.9992$ for $J_1 > 0$, and $J_{1c} \simeq -8.144T + 1.999$ for $J_1 < 0$. All these show again that considerable enhancement of TQD can be achieved by tuning the strength of the inhomogeneous exchange interaction J_1 moderately.

We now discuss TQD for $\rho(T)$ with the bipartition $\{1-23\}$. Here, we compute $D(\rho_{1,23})$ numerically, and the corresponding results are plotted in Fig. 3. As the QD is nonincreasing by tracing out one qubit [11], we have $D(\rho_{1,23}) \geq D(\rho_{1,2})$, which can be certified by comparing Figs. 1 and 3.

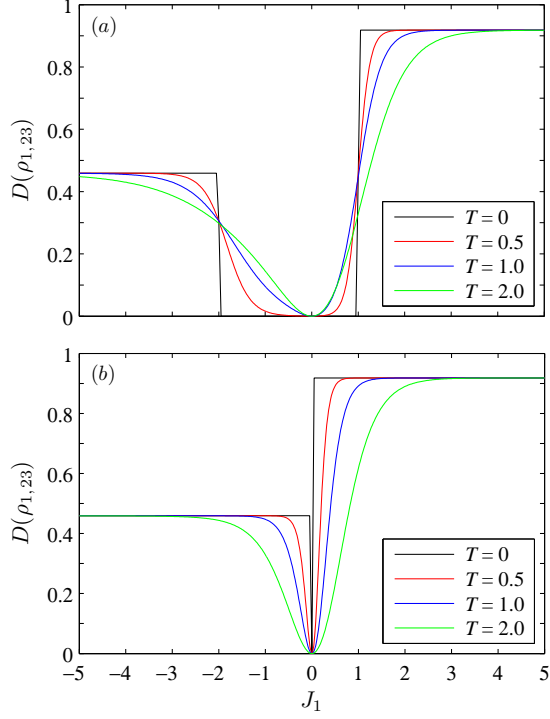


FIG. 3: TQD $D(\rho_{1,23})$ between spin 1 and the spin pair $\{23\}$ versus J_1 with different scaled temperature T , and the parameter J is chosen to be $J = 1$ (a) and $J = -1$ (b), respectively.

At absolute zero temperature with the addition of $J > 0$, we have $D(\rho_{1,23}) \simeq 0.9183$ when $J_1 > J$, $D(\rho_{1,23}) \simeq 0.4591$ when $J_1 < -2J$, and $D(\rho_{1,23}) = 0$ when $J_1 \in (-2J, J)$. If $J < 0$, however, we have $D(\rho_{1,23}) \simeq 0.9183$ (0.4591) when $J_1 > 0$ ($J_1 < 0$). At finite temperature T , the TQD $D(\rho_{1,23})$ shows very similar behaviors with that of $D(\rho_{1,2})$ (see, Fig. 3), i.e., it may be enhanced by increasing the absolute value of J_1 , and when $J_1 \rightarrow \infty$ ($-\infty$) it arrives at the asymptotic value 0.9183 (0.4591). Moreover, the TQD is reduced by increasing temperature of the reservoir except the special case of $J_1 \in (-2J, J)$ and $J > 0$.

B. Magnetic impurity

For this situation, the interactions between the neighboring spins are completely the same, and the magnetic impurity is assumed to be along z -direction of the first spin.

We compute the TQD for different spin pairs numerically, and an exemplified plot was displayed in Fig. 4 with $J = 1$ and $T = 0.25$, from which one can see that with the increasing strength of B , $D(\rho_{23})$ approaches to its maximum 1 asymptotically [$D(\rho_{12})$ with $J > 0$, or $D(\rho_{12})$ and $D(\rho_{23})$ with $J < 0$ are always decreased with increasing B]. By tuning strength of a nonuniform magnetic field located on one spin, one can enhance the TQD between the other two spins. This phenomenon reflects the remarkable nonlocal feature of quantum mechanics.

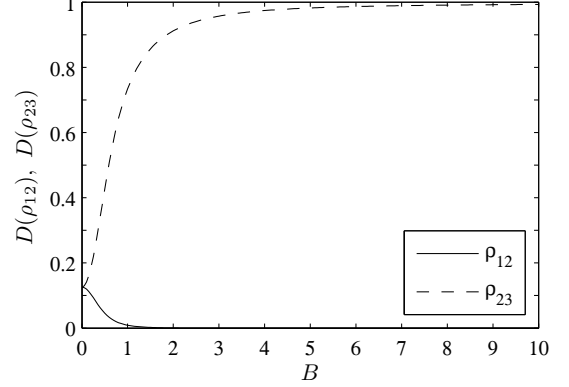


FIG. 4: TQDs $D(\rho_{12})$ and $D(\rho_{23})$ versus the nonuniform magnetic field B (along z -direction of spin 1) with $J = 1$ and $T = 0.25$.

V. SUMMARY

To summarize, we have investigated properties of TQD in the Heisenberg chain, which is assumed to be in thermal equilibrium with a reservoir at temperature T . We considered the case that there are spin site imperfection or magnetic impurity in the chain, and discussed their influence on TQD between the chosen spin pairs. By comparing its behaviors under different system parameters, we showed that just as every coin has two sides, the unwanted effects of the inhomogeneous exchange interaction induced by the spin impurity can be used to improve the TQD greatly for all the bipartite states considered. Moreover, we also showed that for the antiferromagnetic Heisenberg chain with homogeneous exchange interactions, an magnetic impurity along the z -direction of one spin can even be used to make TQD between the other two spins approaching its maximal value 1, which is reminiscent of the nonlocal feature of quantum theory.

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